# High Performance Molecular Dynamics (PATC)
## 18-20th February 2019
### CINECA, Via Magnanelli 6/3, 40033 Casalecchio di Reno (BO)

**Teachers**: Andrew Emerson, Alessandro Grottesi, Neva Besker

**Guest teacher**: Giovanni Bussi, SISSA

## Day 1

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|---|---|
| 9.00 – 9.30 | Registration |
| 9.30 – 11.00 | Introduction to HPC architectures I (A. Emerson) |
| 11.00 – 11.30 | Coffee break |
| 11.30 – 12.30 | Introduction to Classic Molecular Dynamics (A. Grottesi) |
| 12.30 – 14.00 | Lunch break |
| 14.00 – 15.10 | MD: Atom, Force and Domain Decomposition (A. Emerson) |
| 15.10 – 15.30 | Coffee break |
| 15.30 – 17.30 | **Tutorial 1**: UNIX Environment@ CINECA: SLURM scheduler (A. Grottesi) |

## Day 2

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|---|---|
| 9.30 – 10.15 | MD on HPC Architectures: GPU, Intel Xeon KNL, Skylake (A. Grottesi) |
| 10.15 – 11.00 | **Tutorial 2**: MD @ CINECA, scripts and benchmarks (A. Grottesi & N. Besker) |
| 11.00 – 11.30 | Coffee break |
| 11.30 – 12.30 | PLUMED Lecture (G. Bussi) |
| 12.30 – 14.00 | Lunch break |
| 14.00 – 15.30 | **Tutorial 3**: PLUMED (G. Bussi) |
| 15.30 – 16.00 | Coffee break |
| 16.00 – 17.30 | **Tutorial 4**: Scalability test for biological systems (N. Besker and A. Grottesi) |

## Day 3

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|---|---|
| 9.30 – 11.00 | Advanced Molecular Dynamics techniques and benchmarks (A. Emerson & A. Grottesi |
| 11.00 – 11.30 | Coffee break |
| 11.30 – 13.00 | **Tutorial 5**: Running and analysis of MD Trajectories (N. Besker) |
| 13.00 – 14.00 | Lunch Break |
| 14.00 – 14.30 | Access to CINECA HPC resources @ CINECA (A. Emerson) |
| 14.30 – 17.30 | Free exercises and tutorials. |